

University of Groningen

## On the construction of discrete filters for symmetry-preserving regularization models

Trias, F.X.; Verstappen, R.W.C.P.

*Published in:*  
Computers & fluids

*DOI:*  
[10.1016/j.compfluid.2010.08.015](https://doi.org/10.1016/j.compfluid.2010.08.015)

**IMPORTANT NOTE:** You are advised to consult the publisher's version (publisher's PDF) if you wish to cite from it. Please check the document version below.

*Document Version*  
Publisher's PDF, also known as Version of record

*Publication date:*  
2011

[Link to publication in University of Groningen/UMCG research database](#)

*Citation for published version (APA):*

Trias, F. X., & Verstappen, R. W. C. P. (2011). On the construction of discrete filters for symmetry-preserving regularization models. *Computers & fluids*, 40(1), 139-148.  
<https://doi.org/10.1016/j.compfluid.2010.08.015>

**Copyright**

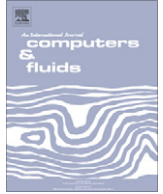
Other than for strictly personal use, it is not permitted to download or to forward/distribute the text or part of it without the consent of the author(s) and/or copyright holder(s), unless the work is under an open content license (like Creative Commons).

The publication may also be distributed here under the terms of Article 25fa of the Dutch Copyright Act, indicated by the "Taverne" license. More information can be found on the University of Groningen website: <https://www.rug.nl/library/open-access/self-archiving-pure/taverne-amendment>.

**Take-down policy**

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

*Downloaded from the University of Groningen/UMCG research database (Pure): <http://www.rug.nl/research/portal>. For technical reasons the number of authors shown on this cover page is limited to 10 maximum.*



# On the construction of discrete filters for symmetry-preserving regularization models

F.X. Trias<sup>a,b,\*</sup>, R.W.C.P. Verstappen<sup>b</sup>

<sup>a</sup> Heat and Mass Transfer Technological Center, Technical University of Catalonia ETSEIAT, c/Colom 11, 08222 Terrassa, Spain

<sup>b</sup> Institute of Mathematics and Computing Science, University of Groningen, P.O. Box 407, 9700 AK Groningen, The Netherlands

## ARTICLE INFO

### Article history:

Received 23 April 2010

Received in revised form 17 August 2010

Accepted 19 August 2010

Available online 26 August 2010

### Keywords:

Filter

Turbulence modeling

Symmetry-preserving

Regularization modeling

Burgers' equation

LES

## ABSTRACT

Since direct numerical simulations cannot be computed at high Reynolds numbers, a dynamically less complex formulation is sought. In the quest for such a formulation, we consider regularizations of the convective term that preserve the symmetry and conservation properties exactly. This requirement yielded a novel class of regularizations [Verstappen R. On restraining the production of small scales of motion in a turbulent channel flow. *Comput Fluids* 2008;37:887–97.] that restrains the convective production of smaller and smaller scales of motion in an unconditionally stable manner, meaning that the velocity cannot blow up in the energy-norm (in 2D also: enstrophy-norm). The numerical algorithm used to solve the governing equations must preserve the symmetry and conservation properties too. To do so, one of the most critical issues is the discrete filtering. The method requires a list of properties that, in general, is not preserved by classical filters for LES unless they are imposed *a posteriori*. In the present paper, we propose a novel class of discrete filters that preserves such properties *per se*. They are based on polynomial functions of the discrete diffusive operator,  $\tilde{D}$ , with the general form  $F = I + \sum_{m=1}^M d_m \tilde{D}^m$ . Then, the coefficients,  $d_m$ , follow from the requirement that, at the smallest grid scale  $k_c$ , the amount by which the interactions between the wavevector-triples  $(k_c, k_c - q, q)$  are damped must become virtually independent of the  $q$ th Fourier-mode. This allows an optimal control of the subtle balance between convection and diffusion at the smallest grid scale to stop the vortex-stretching. Finally, the resulting filters are successfully tested for the Burgers' equation.

© 2010 Elsevier Ltd. All rights reserved.

## 1. Introduction

The incompressible Navier–Stokes (NS) equations form an excellent mathematical model for turbulent flows. In primitive variables the equations are

$$\partial_t u + \mathcal{C}(u, u) = \frac{1}{Re} \Delta u - \nabla p; \nabla \cdot u = 0 \quad (1)$$

where  $u$  denotes the velocity field,  $p$  represents the pressure,  $Re$  is the Reynolds number and the non-linear convective term is defined by  $\mathcal{C}(u, v) = (u \cdot \nabla) v$ .

Preserving the (skew-)symmetries of the continuous differential operators when discretizing them has been shown to be a very suitable approach for direct numerical simulation (DNS) (see [1], for instance). Doing so, certain fundamental properties such as the inviscid invariants – kinetic energy, enstrophy (in 2D) and

helicity (in 3D) – are exactly preserved in a discrete sense. However, direct simulations at high Reynolds numbers are not feasible because the convective term produces far too many relevant scales of motion. Therefore, a dynamically less complex mathematical formulation is needed. In the quest for such a formulation, we consider regularizations [2,3] (smooth approximations) of the nonlinearity. The first outstanding approach in this direction goes back to Leray [4]. The Navier–Stokes- $\alpha$  model also forms an example of regularization modeling (see [3], for instance). The regularization methods basically alter the convective terms to reduce the production of small scales of motion. In doing so, we proposed to preserve exactly the symmetry and conservation properties of the convective terms [5]. This requirement yielded a family of *symmetry-preserving regularization* models: a novel class of regularizations that restrains the convective production of smaller and smaller scales of motion in an unconditionally stable manner, meaning that the velocity cannot blow up in the energy-norm (in 2D also: enstrophy-norm). The numerical algorithm used to solve the governing equations preserves the conservation properties too [1] and is therefore well-suited to test the proposed simulation model. The regularization makes use of a normalized self-adjoint filter. In the initial tests [5,6], the performance of the method was tested

\* Corresponding author at: Heat and Mass Transfer Technological Center, Technical University of Catalonia ETSEIAT, c/Colom 11, 08222 Terrassa, Spain. Tel.: +34 93 739 81 92; fax: +34 93 739 81 01.

E-mail addresses: [cttc@cttc.upc.edu](mailto:cttc@cttc.upc.edu), [xavitrias@gmail.com](mailto:xavitrias@gmail.com) (F.X. Trias), [R.W.C.P.Verstappen@rug.nl](mailto:R.W.C.P.Verstappen@rug.nl) (R.W.C.P. Verstappen).

keeping the ratio  $\epsilon/h$  (filter length/grid width) constant. Thus, this parameter had to be prescribed in advance and therefore a convergence analysis respect to  $\epsilon/h$  was needed. Later, to circumvent this, a parameter-free approach was proposed [7]: the regularization parameter (the local filter length,  $\epsilon$ ) is dynamically determined from the requirement that the vortex-stretching must be stopped at the scale set by the grid. However, in this way, some basic properties of the filter (i.e., symmetry, normalization, incompressibility, etc.) are lost. Therefore, they need to be restored by explicitly forcing them; however, such *a posteriori* modifications are artifacts that may change the dynamics of the system significantly.

In this context, here we propose a family of discrete linear filters that preserves several fundamental properties by construction. To do so, polynomial functions of the discrete diffusive operator,  $\tilde{D}$ , with the general form  $F = I + \sum_{m=1}^M d_m \tilde{D}^m$  are considered. In this way, a list of properties are automatically satisfied *per se*: (i) the filter is exactly symmetric and normalized, (ii) the diffusive nature of the filter implies that there is no introduction of any non-physical transport between scales and (iii) a filtered divergence-free vector remains ‘almost’ incompressible. Moreover, since they are only based on the diffusive operator, their implementation, even for unstructured formulations, becomes straightforward. Then, the exact coefficients,  $d_m$ , follow from the requirement that the damping of all triadic interactions at the smallest scale,  $k_c$ , must become virtually independent of the interacting wavevectors-triples  $(k_c, k_c - q, q)$ . The latter is a crucial property to control the subtle balance between convection and diffusion in order to stop the vortex-stretching mechanism.

The rest of the paper is arranged as follows. In the next section, the symmetry-preserving regularization models are briefly presented. The interscale interactions are studied in detail in the spectral space. The criterion to determine the regularization parameter (i.e., the local filter length) follows from the requirement that the vortex-stretching must stop at the smallest grid scale. Then, the numerical approximations needed to apply the method in a discrete setting are addressed in Section 3. The important role of the discrete operators of the NS equations and the linear filter are discussed. In Section 4, the novel class of discrete filters based on polynomial functions of the discrete diffusive operator is presented and analyzed. Then, in Section 5, the performance of the method is assessed through application to the Burgers’ equation which holds many similarities with the NS equations. Finally, relevant results are summarized and conclusions are given.

## 2. Restraining the production of small scales: $C_n$ -regularization

### 2.1. Regularization modeling

At high  $Re$ -numbers, the velocity field cannot be computed numerically from the NS Eqs. (1), because the solution possesses far too many scales of motion. The computationally almost numberless small scales result from the non-linear convective term  $\mathcal{C}(u, u)$  that allow the transfer of energy from scales as large as the flow domain to the smallest scales that can survive viscous dissipation. In the quest for a dynamically less complex mathematical formulation, we consider smooth approximations (regularizations) of the nonlinearity,

$$\partial_t u_\epsilon + \tilde{\mathcal{C}}(u_\epsilon, u_\epsilon) = \frac{1}{Re} \Delta u_\epsilon - \nabla p_\epsilon; \quad \nabla \cdot u_\epsilon = 0 \quad (2)$$

where the variable names are changed from  $u$  and  $p$  to  $u_\epsilon$  and  $p_\epsilon$ , respectively, to stress that the solution of (2) differs from that of the NS equations.

The regularized system (2) should be more amenable to be solved numerically (meaning that the regularization should limit

the production of small scales of motion), while the leading modes of  $u_\epsilon$  have to approximate the corresponding modes of the solution  $u$  of the NS Eq. (1). The regularized system (2) may also be seen in relation to large-eddy simulation (LES). In LES, Eqs. (1) are filtered spatially, and the resulting nonlinear terms involving residual velocities are modeled in terms of the filtered velocity

$$\partial_t \bar{u}_\epsilon + \mathcal{C}(\bar{u}_\epsilon, \bar{u}_\epsilon) = \frac{1}{Re} \Delta \bar{u}_\epsilon - \nabla p_\epsilon + \mathcal{M}(\bar{u}_\epsilon), \quad (3)$$

where the model terms are approximately given by  $\mathcal{M}(\bar{u}_\epsilon) \approx \mathcal{C}(\bar{u}_\epsilon, \bar{u}_\epsilon) - \overline{\mathcal{C}(u_\epsilon, u_\epsilon)}$ . The regularization described by Eq. (2) falls in this concept if

$$\overline{\mathcal{C}(u_\epsilon, u_\epsilon)} = \mathcal{C}(\bar{u}_\epsilon, \bar{u}_\epsilon) - \mathcal{M}(\bar{u}_\epsilon). \quad (4)$$

Indeed under this condition, Eq. (2) are equivalent to (3): we can filter (2) first and thereafter compare the filtered version of (2) term-by-term with (3) to identify the closure model  $\mathcal{M}(\bar{u}_\epsilon)$ . Finally, it may be noted that Eq. (4) relates the regularization  $\tilde{\mathcal{C}}(u_\epsilon, u_\epsilon)$  one-to-one to the closure model  $\mathcal{M}$  for any invertible filter.

### 2.2. Symmetry-preserving regularization models

The regularization method basically alters the nonlinearity to restrain the production of small scales of motion (see e.g. [3]). In doing so, we propose to exactly preserve certain fundamental symmetry properties of the convective operator  $\mathcal{C}$  in Eq. (1), i.e.

$$(\mathcal{C}(u, v), w) = -(\mathcal{C}(u, w), v), \quad (5)$$

$$(\mathcal{C}(u, v), \Delta v) = (u, \mathcal{C}(\Delta v, v)), \quad (6)$$

where the skew-symmetry with respect to  $v$  and  $w$  of the trilinear form  $(\mathcal{C}(u, v), w)$  ensures the conservation of energy and helicity. Additionally, the identity (6) must be satisfied to conserve enstrophy in 2D. Therefore, we aim to regularize the convective operator  $\mathcal{C}$  in such a manner that the underlying symmetries (given by Eqs. (5) and (6)) are preserved. In other words, we require that the approximation  $\tilde{\mathcal{C}}$  of  $\mathcal{C}$  satisfies  $(\tilde{\mathcal{C}}(u, v), w) = -(\mathcal{C}(u, w), v)$ , and in 2D,  $(\tilde{\mathcal{C}}(u, v), \Delta v) = (u, \mathcal{C}(\Delta v, v))$ . This criterion yields the following class of regularizations proposed in [5],

$$\mathcal{C}_2(u, v) = \mathcal{C}(\bar{u}, \bar{v}), \quad (7a)$$

$$\mathcal{C}_4(u, v) = \mathcal{C}(\bar{u}, \bar{v}) + \overline{\mathcal{C}(\bar{u}, v')} + \overline{\mathcal{C}(u', \bar{v})}, \quad (7b)$$

$$\mathcal{C}_6(u, v) = \mathcal{C}(\bar{u}, \bar{v}) + \mathcal{C}(\bar{u}, v') + \mathcal{C}(u', \bar{v}) + \overline{\mathcal{C}(u', v')}, \quad (7c)$$

where a prime indicates the residual of the filter, e.g.  $u' = u - \bar{u}$ , which can be explicitly evaluated, and  $\overline{(\cdot)}$  represents a normalized self-adjoint linear filter with filter length  $\epsilon$ . The difference between  $\mathcal{C}_n(u, u)$  and  $\mathcal{C}(u, u)$  is of order  $\epsilon^n$  (where  $n = 2, 4, 6$ ) for symmetric filters with filter length  $\epsilon$ . Note that for a generic, symmetric filter:  $u' = \mathcal{O}(\epsilon^2)u$  (see e.g. [8]).

The approximations  $\mathcal{C}_n(u_\epsilon, u_\epsilon)$  are stable by construction, meaning that convective terms do not contribute to the evolution of  $|u_\epsilon|^2$ ; hence, the evolution of  $|u_\epsilon|^2$  is governed by a dissipative process. Therefore, replacing the convective term in the NS equations by the  $\mathcal{O}(\epsilon^n)$ -accurate smooth approximation  $\mathcal{C}_n(u_\epsilon, u_\epsilon)$ , the partial differential equations to be solved result in

$$\partial_t u_\epsilon + \mathcal{C}_n(u_\epsilon, u_\epsilon) = \frac{1}{Re} \Delta u_\epsilon - \nabla p_\epsilon; \quad \nabla \cdot u_\epsilon = 0. \quad (8)$$

For further details about the symmetry-preserving regularization modeling the reader is referred to [5].

### 2.3. Triadic interactions

To study the interscale interactions in more detail, we continue in the spectral space. The spectral representation of the convective term in the NS equations is given by

$$\mathcal{C}(u, v)_k = i\Pi(k) \sum_{p+q=k} \hat{u}_p \hat{v}_q, \quad (9)$$

where  $\Pi(k) = I - k k^T / |k|^2$  denotes the projector onto divergence-free velocity fields in the spectral space. Taking the Fourier transform of 7a, 7b and 7c, we obtain the evolution of each Fourier-mode  $\hat{u}_k(t)$  of  $u_\epsilon(t)$  for the  $\mathcal{C}_n$  approximation<sup>1</sup>

$$\left( \frac{d}{dt} + \frac{1}{Re} |k|^2 \right) \hat{u}_k + i\Pi(k) \sum_{p+q=k} f_n(\hat{g}_k, \hat{g}_p, \hat{g}_q) \hat{u}_p \hat{u}_q = F_k, \quad (10)$$

where  $\hat{g}_k$  denotes the  $k$ th Fourier-mode of the kernel of the convolution filter, i.e.,  $\hat{u}_k = \hat{g}_k \hat{u}_k$ . The mode  $\hat{u}_k$  interacts only with those modes whose wavevectors  $p$  and  $q$  form a triangle with the vector  $k$ . Thus, compared with (9), every triad interaction is multiplied by

$$f_2(\hat{g}_k, \hat{g}_p, \hat{g}_q) = \hat{g}_k \hat{g}_p \hat{g}_q, \quad (11a)$$

$$f_4(\hat{g}_k, \hat{g}_p, \hat{g}_q) = \hat{g}_k \hat{g}_p + \hat{g}_k \hat{g}_q + \hat{g}_p \hat{g}_q - 2\hat{g}_k \hat{g}_p \hat{g}_q, \quad (11b)$$

$$f_6(\hat{g}_k, \hat{g}_p, \hat{g}_q) = 1 - (1 - \hat{g}_k)(1 - \hat{g}_p)(1 - \hat{g}_q). \quad (11c)$$

Moreover, since for a generic symmetric convolution filter (see [8], for instance),  $\hat{g}_k = 1 - \alpha^2 |k|^2 + \mathcal{O}(\alpha^4)$  with  $\alpha^2 = \epsilon^2/24$ , the damping functions  $f_n$  can be approximated by

$$f_2 \approx 1 - \alpha^2 (|k|^2 + |p|^2 + |q|^2), \quad (12a)$$

$$f_4 \approx 1 - \alpha^4 (|k|^2 |p|^2 + |k|^2 |q|^2 + |p|^2 |q|^2), \quad (12b)$$

$$f_6 \approx 1 - \alpha^6 |k|^2 |p|^2 |q|^2. \quad (12c)$$

Therefore, the interactions between large scales of motion ( $\epsilon |k| < 1$ ) approximate the NS dynamics up to  $\mathcal{O}(\epsilon^n)$  with  $n = 2, 4, 6$ , respectively. Hence, the triadic interactions between large scales are only slightly altered. All interactions involving longer wavevectors (smaller scales of motion) are reduced. The amount by which the interactions between the wavevector-triple  $(k, p, q)$  are lessened depends on the length of the legs of the triangle  $k = p + q$ . In the case  $n = 4$ , for example, all triadic interactions for which at least two legs are (much) longer than  $1/\epsilon$  are (strongly) attenuated; whereas, interactions for which at least two legs are (much) shorter than  $1/\epsilon$  are reduced to a small degree only.

### 2.4. Stopping the vortex-stretching mechanism

In the initial tests, the performance of the  $\mathcal{C}_4$  approximation was tested keeping the ratio  $\epsilon/h$  (filter length to the grid width) constant. Therefore, only one parameter needed to be prescribed in advance. Later, to circumvent this, a parameter-free approach was proposed [7]. To do so, we determine the regularization parameter (the local filter length) dynamically from the requirement that the vortex-stretching must be stopped at the smallest scale set by the grid,  $k_c = \pi/h$ . Shortly, the idea behind is to modify the convective operator sufficiently to guarantee that the following inequality is hold

$$\frac{\omega_{k_c} \cdot \mathcal{C}_n(\omega, u)_{k_c}}{\omega_{k_c} \cdot \omega_{k_c}} \leq \frac{1}{Re} k_c^2. \quad (13)$$

In this way, vortex-stretching is restrained enough to prevent a local intensification of vorticity. Then, recalling the evolution Eq. (10) of the  $k$ th Fourier-mode for the  $\mathcal{C}_n$ -approximation, the previous expression becomes

$$\frac{\omega_{k_c} \cdot \left( \sum_{p+q=k_c} f_n(\hat{g}_{k_c}, \hat{g}_p, \hat{g}_q) \hat{u}_p \hat{u}_q \right)}{\omega_{k_c} \cdot \omega_{k_c}} \leq \frac{1}{Re} k_c^2. \quad (14)$$

Note that  $f_n(\hat{g}_{k_c}, \hat{g}_p, \hat{g}_q)$  depends on the filter length  $\epsilon$  and, in general, on the wavevectors  $p$  and  $q = k_c - p$ . This makes very difficult to control the overall damping effect because  $f_n$  cannot be taken out of the summation. To avoid this, filters should be constructed from the requirement that the damping effect of all the triadic interactions at the smallest scale must be virtually independent of the interacting pairs, i.e.

$$f_n(\hat{g}_{k_c}, \hat{g}_p, \hat{g}_q) \approx f_n(\hat{g}_{k_c}). \quad (15)$$

This is a crucial property to control the subtle balance between convection and diffusion in order to stop the vortex-stretching mechanism.

## 3. Playing with discrete operators

The regularizations  $\mathcal{C}_n$  given by Eqs. 7a, 7b and 7c are constructed in a way that the symmetry properties (5) and (6) are exactly preserved. Of course, the same should hold for the numerical approximations that are used to discretize them. For this, the basic ingredients are twofold: (i) the original NS equations must be discretized preserving the symmetries of the continuous differential operators and (ii) a normalized self-adjoint linear filter.

### 3.1. Symmetry-preserving discretization of NS equations

Preserving the symmetries of the continuous differential operators when discretizing them has been shown to be a very suitable approach for DNS of incompressible flows [1]. In short, the temporal evolution of the spatially discrete staggered velocity,  $u_h$ , is governed by the following finite-volume discretization of Eq. (8)

$$\Omega \frac{du_h}{dt} + C(u_h)u_h + Du_h - M^T p_h = 0_h, \quad (16)$$

where the discrete incompressibility constraint reads  $M u_h = 0_h$ . The diffusive matrix,  $D$ , is symmetric and positive semi-definite; it represents the integral of the diffusive flux  $-\nabla u \cdot n / Re$  through the faces. The diagonal matrix,  $\Omega$ , describes the sizes of the control volumes and the approximate, convective flux is discretized as in [1]. The resulting convective matrix,  $C(u_h)$ , is skew-symmetric, i.e.  $C(u_h) + C^T(u_h) = 0$ . In a discrete setting, the skew-symmetry of  $C(u_h)$  implies that

$$C(u_h)v_h \cdot w_h = v_h \cdot C^T(u_h)w_h = -v_h \cdot C(u_h)w_h, \quad (17)$$

for any discrete velocity vectors  $u_h$  (if  $M u_h = 0_h$ ),  $v_h$  and  $w_h$ . Note that Eq. (17) is the discrete analogue of Eq. (5). Then, the evolution of the discrete energy,  $\|u_h\|^2 = u_h \cdot \Omega u_h$ , is governed by

$$\frac{d}{dt} \|u_h\|^2 = -u_h \cdot (D + D^T)u_h < 0, \quad (18)$$

where the convective and pressure gradient contributions cancel because of Eq. (17) and incompressibility constraint  $M u_h = 0_h$ , respectively. Therefore, even for coarse grids, the energy of the resolved scales of motion is convected in a stable manner: that is, the discrete convective operator transports energy from a resolved scale of motion to other resolved scales without dissipating any energy, as it should do from a physical point-of-view. This forms a good starting point for LES-like simulations (see [9], for instance). For a detailed explanation, the reader is referred to [1].

<sup>1</sup> Here, for simplicity, the subindex  $\epsilon$  is dropped.

### 3.2. Discrete filtering

Filtering is usually done by means of an integral operator with a symmetrical convolution kernel. In a discrete setting, this results into a linear operator  $\tilde{u}_h = \tilde{F}u_h$ . However, to constitute a suitable filter,  $\tilde{u}_h = Fu_h$  where  $F \approx \tilde{F}$ , for our application, the following basic properties are required:

- (i) Symmetry,  $\Omega F = (\Omega F)^T$ .
- (ii) Normalization, i.e. constant velocity vector is unaffected,  $F1 = 1$ .
- (iii) Given an incompressible velocity field,  $u_h$  ( $Mu_h = 0_h$ ),  $\tilde{u}_h$  must be also divergence-free.
- (iv) Low-pass filtering, i.e. only high-frequency components must be effectively damped.
- (v) The damping effect of  $f_n(\tilde{g}_k, \tilde{g}_p, \tilde{g}_q)$  must be virtually independent of the interacting pair ( $p, q = k_c - p$ ); that is Eq. (15) need to be satisfied.

The first three properties are required to ensure that all the symmetry and conservation properties hold exactly [5]. However, in general, they are not satisfied by  $\tilde{F}$ ; therefore, we need to redefine our linear filter  $F$  as follows

$$F = S - \text{diag}(S1 - 1) \text{ with } 2S = \Omega^{-1} \{ \Omega \tilde{F} + (\Omega \tilde{F})^T \}. \quad (19)$$

Then, the linear map  $u_h \mapsto \tilde{u}_h$  defined by Eq. (19) possesses the basic properties (i) and (ii). Then, regarding the point (iii), it must be noted that in general an incompressible velocity field,  $u_h$  ( $Mu_h = 0_h$ ), does not automatically imply that  $\tilde{u}_h$  ( $u'_h = u_h - \tilde{u}_h$  also) is also divergence-free. Although no ‘real’ mass is lost in terms of the  $u_h$  field,  $M\tilde{u}_h \neq 0_h$  and  $M\tilde{u}'_h \neq 0_h$  have series implications: the skew-symmetry of the convective operator (17) and consequently the conservation properties that follow from it would be lost. For instance, because of this, the convection term would not be a pure redistributor of energy any more; instead, it becomes an active source or sink of kinetic energy and therefore the stability of the method is lost. This question has been addressed before for a Leray- $\alpha$  model in [10]. One possible solution to this problem could be to project the filtered velocity,  $\tilde{u}_h$ , onto a divergence-free space,

$$\tilde{u}_h = Fu_h, \quad (20)$$

$$\tilde{u}_h^p = \tilde{u}_h + \Omega^{-1} M^T q_h \text{ with } M\tilde{u}_h^p = 0_h. \quad (21)$$

However, an additional Poisson equation,  $-M\Omega^{-1} M^T q_h = M\tilde{u}_h$ , needs to be solved each time-step. A computationally less demanding approach relies on explicitly forcing the diagonal term of the discrete convective operators,  $C(u_h)$ , to be equal to zero,

$$[C(u_h)]_{jj} = 0 \quad \forall j. \quad (22)$$

In this way, the skew-symmetry of the convective operator (17) is restored irrespective whether the advective velocity is exactly divergence-free. Both approaches have been tested in [7]. Since no significant differences have been observed, in the view of lower costs, the second approach was chosen.

Assuming that the property (iv) is also satisfied, we can conclude that  $F$  constitutes a suitable filter for our application. However, modifications proposed in Eqs. (19) and (22) are artifacts that may change the dynamics of the system significantly. This problem becomes especially relevant in the near-wall regions where the non-slip boundary conditions may cause significant compressibility effects on the filtered velocity. Finally, regarding the last property (v) it must be satisfied via the adjustment of the convolution kernel of the linear filter. This is addressed in the following section.

### 4. Constructing the discrete filter

As stated above, a list of properties are required to the linear filter,  $F$ , to be suitable for our application. However, they are not satisfied by classical filters for LES and therefore, they need to be imposed *a posteriori* via Eqs. (19) and (22). Alternatively, here we propose a novel family of discrete linear filters that preserve the required properties (i)–(iv) by construction. Then, the exact form follows from the last requirement (v), i.e. the damping effect  $f(\tilde{g}_k, \tilde{g}_p, \tilde{g}_q)$  must be almost independent of the interacting wave-vectors,  $q$  and  $p = k_c - q$ .

#### 4.1. Playing with the discrete diffusive operator, $D$

Here, we propose to construct symmetric linear filters with the general form

$$F = I + \sum_{m=1}^M d_m \tilde{D}^m \text{ with } \tilde{D} = \Omega^{-1} D, \quad (23)$$

where the boundary conditions that supplement the NS Eqs. (1) are applied in (23) too. Then, the convolution kernel of the filter results

$$\hat{G}_k = 1 + \sum_{m=1}^M d_m \hat{D}_k^m, \quad (24)$$

where  $\hat{D}_k$  denotes the transfer function of discrete diffusive operator,  $\tilde{D}$ . In this way, all the above-mentioned basic properties (i)–(iii) are automatically satisfied. Shortly, properties (i) and (ii) follow from the symmetry  $D = D^T$  and the fact that the unity vector lies on the kernel of  $D$ , i.e.  $D1 = 0$  (see [1] for details). Therefore, modification proposed in Eq. (19) is not needed any more. Then, recalling that  $\Delta u = \nabla(\nabla \cdot u) - \nabla \times (\nabla \times u)$ , it follows that  $\nabla \cdot \Delta u = 0$  if  $\nabla \cdot u = 0$  and therefore the property (iii) is also satisfied. In a discrete sense, the latter holds only approximately. Hence, the modification given by (22) is still required.

Furthermore, since they are only based on  $D$  and no additional operator is needed, the method is: (i) easy-to-implement, (ii) boundary conditions are already prescribed in the definition of  $D$ , (iii) the diffusive nature of the filter implies that there is no introduction of any non-physical transport between scales and (iv) from a parallel point-of-view the construction of filters with large stencils ( $M > 1$ ) is straightforward. Then, hereafter the only thing that remains is to determine the values of the coefficients,  $d_m$ , from the requirement that properties (iv) and (v) must be also satisfied. Therefore the influence of the choice of the filter  $\hat{G}_k$  on the so-called bandwidth of  $f_n$  has been further analyzed. We restrict ourselves to the  $\mathcal{C}_4$  approximation. Here, the analysis will be restricted to the case of 1D filters, without the loss of generality.

#### 4.2. Starting point: 3-point filter

When considering a discrete 3-point symmetric filter in physical space, the associated transfer function is given by  $\hat{g}_k = c_0 + 2c_1 \cos(kh)$  where  $h$  is the grid width. Therefore, the transfer function of the classical 3-point diffusive operator ( $c_0 = -2/h^2$  and  $c_1 = 1/h^2$ ) reads

$$\hat{D}_k = \frac{2}{h^2} (\cos(kh) - 1). \quad (25)$$

To simplify the analysis, hereafter we consider  $h = 1$ . Then, the 3-point filter ( $M = 1$ ) becomes  $\hat{G}_k = (1 - 2d_1) + 2d_1 \cos(k)$  where the  $d_1$  is given by

$$d_1 = \frac{1}{4} - \frac{\hat{G}_\pi}{4}. \quad (26)$$



Note that for  $h = 1$  the smallest scale is  $\pi$  (see Fig. 1). Since for  $\mathcal{C}_4$ ,  $f(\hat{G}_\pi, \hat{G}_p, \hat{G}_q) = \hat{G}_\pi(\hat{G}_p + \hat{G}_q) + \hat{G}_p\hat{G}_q(1 - 2\hat{G}_\pi)$  (see Eq. (11b) and  $p = \pi - q$ , the damping function  $f_4$  for the 3-point filter is bounded by

$$f_4^{3p}(\hat{G}_\pi, 0) = -\hat{G}_\pi^2 + 2\hat{G}_\pi, \quad (27)$$

$$f_4^{3p}(\hat{G}_\pi, \pi/2) = -\frac{1}{2}\hat{G}_\pi^3 + \frac{1}{4}\hat{G}_\pi^2 + \hat{G}_\pi + \frac{1}{4}, \quad (28)$$

where the superindex  $3p$  means that the 3-point filter is being used to compute the damping function  $f_4$ . Hereafter, the same notation will be also used for the 5- and 7-point filters. Fig. 2 shows the bandwidth of  $f_4^{3p}(\hat{G}_\pi, q)$  for  $0 \leq \hat{G}_\pi \leq 1$ . For  $1/2 \leq \hat{G}_\pi \leq 1$ , it is small and therefore for these values of  $\hat{G}_\pi$ ,  $f_4^{3p}$  can be taken out of the summation (14). However, for  $\hat{G}_\pi \leq 1/2$ , the bandwidth of  $f_4^{3p}$  increases, and the 3-point filter is no longer satisfactory for taking outside of the summation (14).

#### 4.3. Minimizing the bandwidth of $f_4(\hat{G}_\pi, q)$

Since for the 3-point filter, the coefficient  $d_1$  is given by the condition (26), the bandwidth is fixed. However, additional degrees of freedom, i.e.  $d_2, d_3, \dots$ , may be used to minimize the bandwidth of  $f_4$ . In Appendix A, the discrete 5- and 7-point filters have been deduced. The resulting expression for the 5-point filter ( $M = 2$ ) is given by

$$d_{1,opt} = -\frac{\hat{G}_\pi - 1}{2(2\hat{G}_\pi + 1)}, \quad d_{2,opt} = \frac{2\hat{G}_\pi^2 - 3\hat{G}_\pi + 1}{16(2\hat{G}_\pi + 1)}. \quad (29)$$

Then, taking  $d_2 = d_{2,opt}$  and  $d_1 = d_{1,opt}$ ,  $f_4^{5p}$  is again bounded by  $q = 0$  and  $q = \pi/2$ . Fig. 3 (top) shows the bandwidth of  $f_4^{5p}(\hat{G}_\pi, q, d_{2,opt})$ . However, the bandwidth of  $f_4^{5p}$  for small values of  $\hat{G}_\pi$  may not be small enough. To solve this, an additional degree of freedom is required. Then, the following 7-point filter ( $M = 3$ ) follows

$$\left. \begin{aligned} d_{3,opt} &= \frac{1}{54} \left( \frac{E(\hat{G}_\pi)}{C(\hat{G}_\pi)} + \frac{D(\hat{G}_\pi)}{E(\hat{G}_\pi)} - \frac{7}{2} \right) (\hat{G}_\pi - 1) \\ d_{2,opt} &= 6d_{3,opt} + \frac{1}{2} \sqrt{-8d_{3,opt}^2 - 2d_{3,opt}\hat{G}_\pi + 2d_{3,opt}} \\ d_{1,opt} &= \frac{1}{4} (1 + 16d_{2,opt} - 64d_{3,opt} - \hat{G}_\pi) \end{aligned} \right\}, \quad \text{if } 0 \leq \hat{G}_\pi < 1/2 \quad (30)$$

$$d_{1,opt} = -\frac{\hat{G}_\pi - 1}{2(2\hat{G}_\pi + 1)}, \quad d_{2,opt} = \frac{2\hat{G}_\pi^2 - 3\hat{G}_\pi + 1}{16(2\hat{G}_\pi + 1)}, \quad \text{if } 1/2 \leq \hat{G}_\pi \leq 1 \quad (31)$$

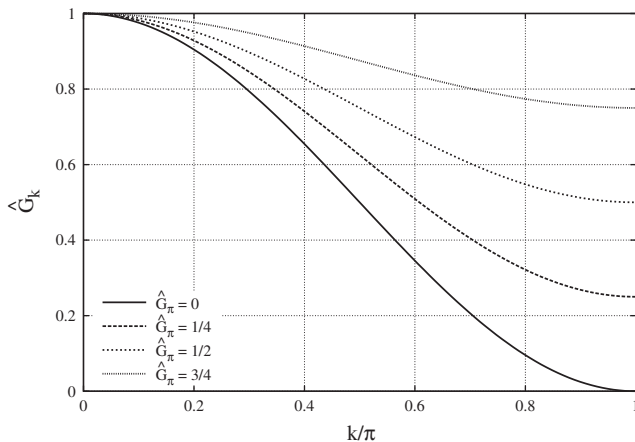


Fig. 1. Transfer function,  $\hat{G}_k$ , for the discrete 3-point filter.

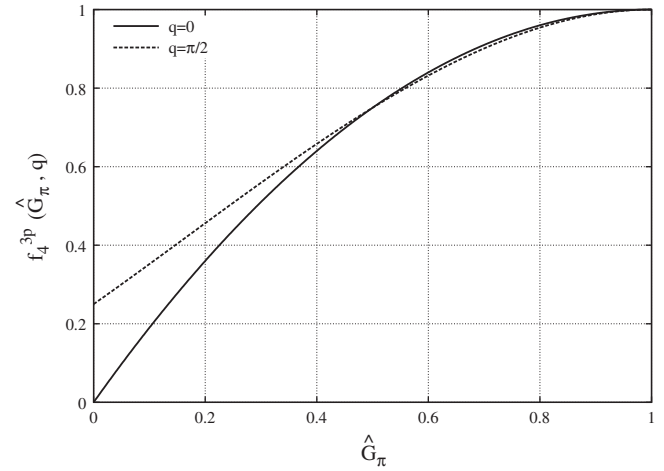


Fig. 2. Bandwidth for  $f_4^{3p}(\hat{G}_\pi, q)$  for the discrete 3-point filter.

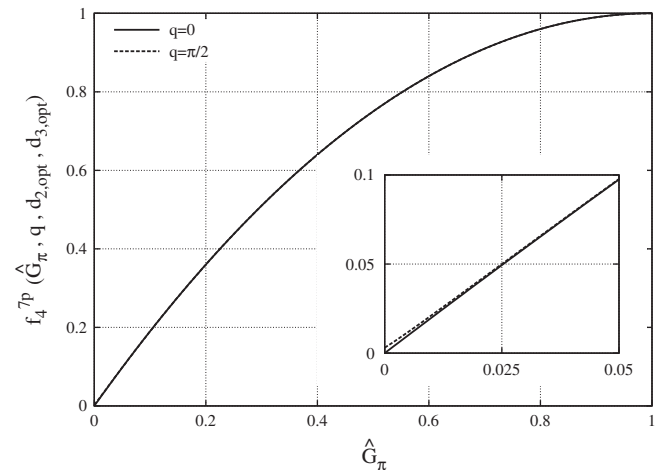
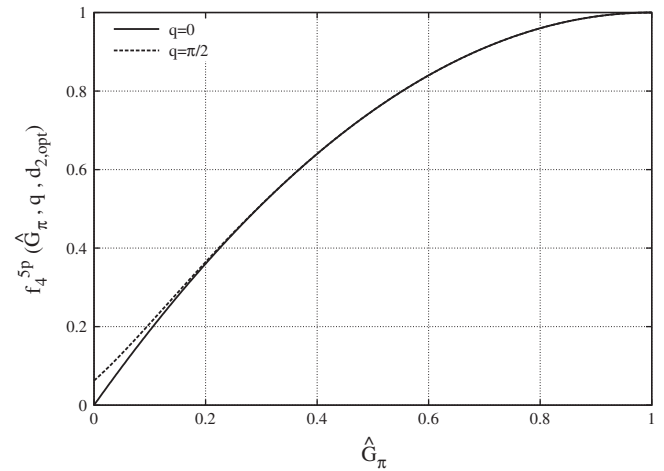


Fig. 3. Bandwidth for  $f_4^{5p}(\hat{G}_\pi, q, d_{2,opt})$  (top) and  $f_4^{7p}(\hat{G}_\pi, q, d_{2,opt}, d_{3,opt})$  (bottom) for the discrete 5-point and 7-point filter, respectively.

where  $C(\hat{G}_\pi)$ ,  $D(\hat{G}_\pi)$  and  $E(\hat{G}_\pi)$  are given by Eqs. 65a, 65bb and 65c (see Appendix A). Note that for  $\hat{G}_\pi \geq 1/2$ , it becomes the 5-point filter given by (29) with a smooth transition from  $f_4^{5p}$  to  $f_4^{7p}$  at  $\hat{G}_\pi = 1/2$ . Fig. 3 (bottom) shows the bandwidth of  $f_4^{7p}(\hat{G}_\pi, q, d_{2,opt}, d_{3,opt})$ . Again,  $f_4^{7p}$  is bounded by  $q = 0$  and  $q = \pi/2$ . Now, the

bandwidth is small for the whole range  $0 \leq \hat{G}_\pi \leq 1$  and therefore  $f_4^{7p}$  can always be taken out of the summation (14).

## 5. Burgers' equation

To test the performance of the new family of filters in conjunction with the  $\mathcal{C}_4$  regularization method we consider the 1D Burgers' equation

$$\partial_t u + \mathcal{C}(u, u) = \frac{1}{Re} \partial_{xx}^2 u + f, \quad (32)$$

on an interval  $\Omega$  with periodic boundary conditions. Despite its simplicity important aspects of the 3D Navier–Stokes equations remain (see [11], for instance). Note that now the convective term is given by  $\mathcal{C}(u, u) = u \partial_x u$ . In Fourier space, it reads

$$\partial_t \hat{u}_k + \mathcal{C}(\hat{u}, \hat{u})_k = -\frac{k^2}{Re} \hat{u}_k + F_k, \quad (33)$$

where  $\hat{u}_k$  denotes the  $k$ th Fourier mode of  $u(x, t) \in \mathbb{R}$  and the non-linear term reads

$$\mathcal{C}(\hat{u}, \hat{u})_k = \sum_{p+q=k} \hat{u}_p i q \hat{u}_q. \quad (34)$$

A forward Euler scheme has been used as time-integration method. Following the same notation than in [12], it reads

$$\frac{[\hat{u}_k]^{n+1} - [\hat{u}_k]^n}{\delta t} = [W_k]^n, \quad (35)$$

where the time-step,  $\delta t$ , is chosen to keep the time-integration numerically stable and  $W_k = -\mathcal{C}(\hat{u}, \hat{u})_k - (k^2/Re)\hat{u}_k$ . Therefore, the discrete time evolution of energy,  $(e_k^{n+1} - e_k^n)/\delta t$ , is given by

$$\frac{[\hat{u}_k]^{n+1} [\hat{u}_k]^{n+1} - [\hat{u}_k]^n [\hat{u}_k]^n}{\delta t} = [\hat{u}_k]^n [W_k]^n + [\hat{u}_k]^n [W_k^*]^n + \delta t [W_k]^n [W_k^*]^n. \quad (36)$$

In Fourier space the regularized convective term is given by

$$\mathcal{C}_4(\hat{u}, \hat{v})_k = \sum_{p+q=k} f_4(\hat{G}_k, \hat{G}_p, \hat{G}_q) \hat{u}_p i q \hat{v}_q, \quad (37)$$

where  $f_4(\hat{G}_k, \hat{G}_p, \hat{G}_q) = \hat{G}_k(\hat{G}_p + \hat{G}_q) + \hat{G}_p \hat{G}_q(1 - 2\hat{G}_k)$  (see Eq. (11b)). Then, to stop the production of smaller scales of motion, the inequality  $\partial_t e_{k_c} \leq 0$  must be satisfied, i.e.

$$[\hat{u}_{k_c}^*]^n [W_{k_c}]^n + [\hat{u}_{k_c}^*]^n [W_{k_c}^*]^n + \delta t [W_{k_c}]^n [W_{k_c}^*]^n \leq 0, \quad (38)$$

where  $k_c$  is the smallest scale. However, such a condition is difficult to be exactly satisfied. In general, the damping function  $f_4(\hat{G}_{k_c}, \hat{G}_p, \hat{G}_q)$  depends on  $p$  and  $q$ ; therefore, the terms in the summation are damped differently. To avoid this, we need to assume that  $f_4(\hat{G}_{k_c}, \hat{G}_p, \hat{G}_q) \approx \tilde{f}_4(\hat{G}_{k_c})$  is almost independent of  $p$  and  $q$ . Then, the value of the function  $f_4$  follows from the requirement that condition (38) must be satisfied. This yields the following quadratic equation for  $\tilde{f}_4$

$$A(\hat{u})(\tilde{f}_4)^2 + B(\hat{u})\tilde{f}_4 + C(\hat{u}) = 0, \quad (39)$$

where  $A(\hat{u}) = \delta t (\mathcal{C}(\hat{u}, \hat{u})_{k_c} \mathcal{C}^*(\hat{u}, \hat{u})_{k_c})$ ,  $B(\hat{u}) = (\hat{u}_{k_c}^* \mathcal{C}(\hat{u}, \hat{u})_{k_c} + \hat{u}_{k_c} \mathcal{C}^*(\hat{u}, \hat{u})_{k_c}) / (\delta t k_c^2 / Re - 1)$  and  $C(\hat{u}) = (\hat{u}_{k_c}^* \hat{u}_{k_c}) k_c^2 / Re (\delta t k_c^2 / Re - 2)$ . In this way, we can guarantee that if the bandwidth of  $f_4$  vanishes, the time-evolution of the energy at the smallest scale,  $e_{k_c}$ , is monotonically decreasing. However, the identity (15) cannot be exactly satisfied. Hence, here we aim to minimize enough the bandwidth of  $f_4$  not to affect significantly the solution. With this in mind, a family of discrete linear filters have been proposed in Section 4.3. Here, the performance of such filters is tested for a Burgers' equation at  $Re = 100$ .

### 5.1. Solution of Burgers' equation at $Re = 100$

The  $\mathcal{C}_4$  approximation has been used to solve the Burgers' equation with  $Re = 100$  and  $\hat{u}_k = k^{-1}$  as initial condition. The forcing term vanishes  $F_k = 0$  for  $k > 1$  and  $F_1$  forces  $\partial_t \hat{u}_1 = 0$ . Fig. 4, shows the energy spectrum of the steady-state solution. Results obtained with and without regularization method for  $k_c = 34$  are compared with a DNS reference spectrum with  $k_c = 200$ . The 7-point filter has been used to compute the  $\mathcal{C}_4$  model. Clearly, the direct simulation without model with  $k_c = 34$  is not able to capture the physics. At high wavenumbers, the energy is not dissipated enough and therefore is reflected back towards the larger scales. The zoom in Fig. 4 shows that the direct simulation with  $k_c = 34$  is already substantially different of the DNS reference solution for  $k = 6$ . The  $\mathcal{C}_4$  solution exhibit one of the features of the model: due to the energy conservation, the model solution displays an additional hump in the spectrum. This was already observed in [5] for a turbulent channel flow. Fig. 5 displays essentially the same for  $k_c = 30, 40, 50$  and  $60$ . As expected, the  $\mathcal{C}_4$  solution of the leading modes becomes closer to the DNS reference solution when  $k_c$  increases. Note

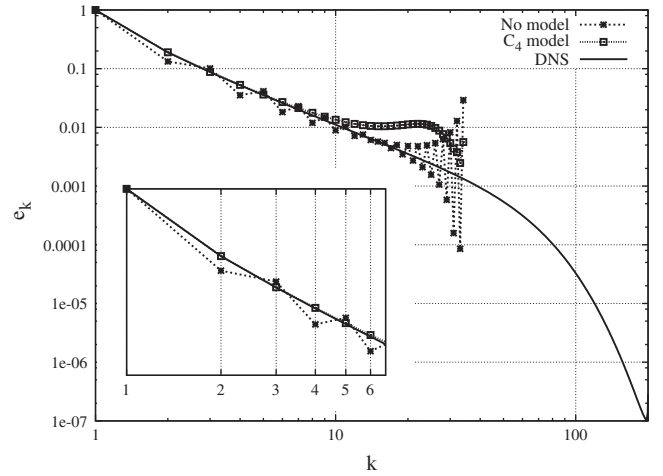


Fig. 4. Energy spectrum of the steady-state solution of the Burgers' equation with and without modeling, for  $k_c = 34$ . Direct comparison with DNS reference solution (solid line), with  $k_c = 200$ .

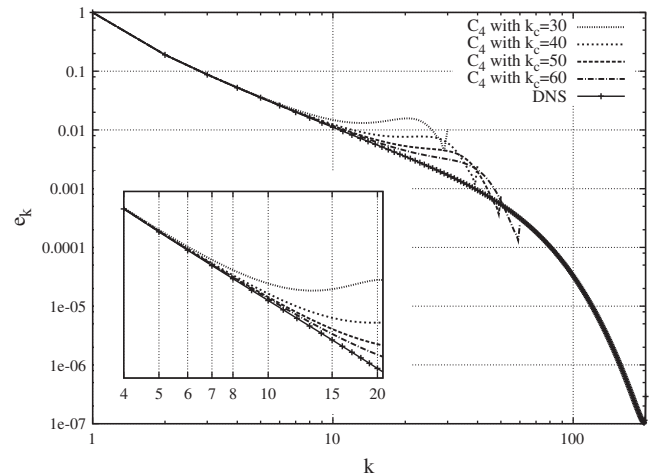
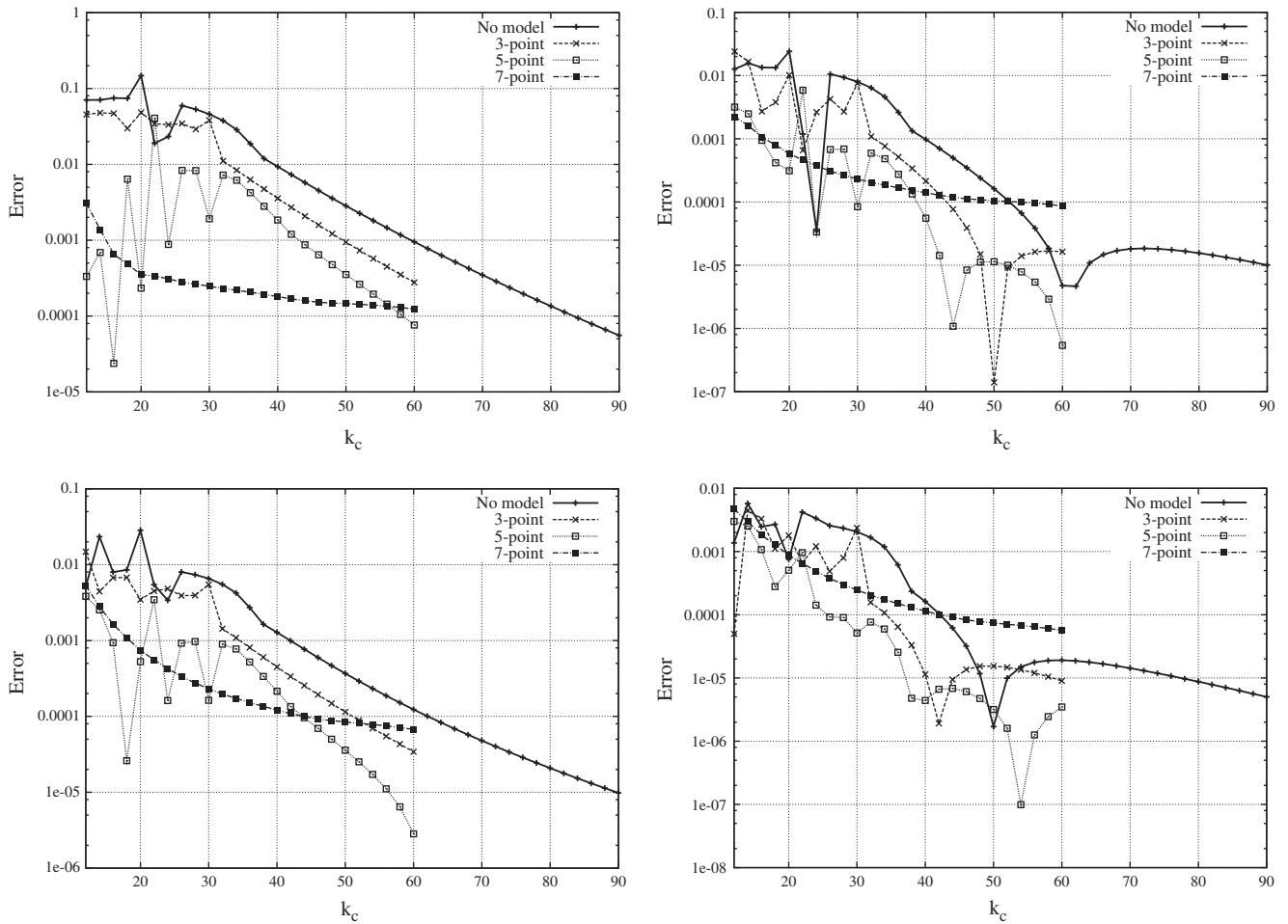


Fig. 5. Energy spectrum of the steady-state solution of the Burgers' equation with  $\mathcal{C}_4$  for  $k_c = 30, 40, 50$  and  $60$ . Direct comparison with DNS reference solution (solid line), with  $k_c = 200$ .



**Fig. 6.** Error versus the total number of nodes,  $k_c$ , for the first four non-fixed modes, i.e.  $k = 2$  (top left),  $k = 3$  (top right),  $k = 4$  (bottom left) and  $k = 5$  (bottom right).

that, due to the non-zero bandwidth of  $f_4^{7p}$ , the energy still tends to pile-up at the smallest scale. However, it seems that the bandwidth of the 7-point filter is small enough not to affect negatively the numerical solution.

To investigate further the influence of  $\mathcal{C}_4$  regularization method together with the family of discrete filters here proposed, a convergence analysis has been performed for the steady-state energy spectrum. Fig. 6 shows the errors respect  $k_c$  for the first four non-fixed modes, i.e.  $k = 2, 3, 4$  and 5. Errors have been measured by direct comparison with a DNS reference solution with  $k_c = 300$ . At first sight, we can observe that the  $\mathcal{C}_4$  method outperforms the direct simulation without modeling, irrespective of the linear filter. However, as expected, the 3-point filter is not able to control the balance between convection and diffusion at the smallest grid scale. Consequently, part of the energy is still reflected back and therefore affects negatively the performance of the method. To tackle such a problem, the 5- and 7-point filters have been proposed in this paper. In general, the 7-point filter clearly performs better for very coarse meshes when this effect becomes more significant. More importantly, the solution using the 7-point filter seems to converge monotonically even for very coarse meshes, whereas the 5-point filter still displays an erratic behavior. It must be noted that for (very) fine resolutions the results obtained with the 7-point filter become worse. However, for such meshes the errors have already reached very low values and therefore, they are not especially significant. A possible explanation for such a behavior could be that for such meshes the role of the model for the lowest frequency modes becomes very small (in

Fig. 6 only the four lowest modes are represented). Under these conditions the dynamical behavior of the system when using the 3- or the 5-point filter converges faster towards the original Burgers' equation. In any case, from a practical point-of-view, these errors are not significant.

## 6. Concluding remarks

The regularizations  $\mathcal{C}_n$  given by Eqs. 7a, 7b and 7c are constructed in a way that the symmetry properties (5) and (6) are exactly preserved. Consequently, the non-linear term  $\mathcal{C}_n(u_\epsilon, u_\epsilon)$  in Eq. (8) redistributes the energy among the various scales of motion without introducing any non-physical dissipation. The production of smaller and smaller scales of motion is regulated by means of a gradual reduction of the energy flux and therefore the energy cascade stops at shorter wavevectors than the original NS equations. At the smallest grid scale, dissipation should be strong enough to stop the energy cascade. This subtle balance between convection and diffusion is ultimately controlled by means of a normalized self-adjoint linear filter. In a discrete setting, the above-mentioned symmetries must be also preserved. This has serious implications for the discrete filter: it must possess a list of properties that, in general, is not satisfied by classical filters for LES unless they are imposed *a posteriori*. However, this is an artifact that may change the dynamics of the system significantly.

In this context, a family of discrete linear filters that preserve the required list of properties by construction has been proposed.



They are based on polynomial functions of the discrete diffusive operator,  $\hat{D}$ , with the general form  $F = I + \sum_{m=1}^M d_m \hat{D}^m$ . In this way, a list of properties is automatically satisfied *per se*: (i) the filter is exactly symmetric and normalized, (ii) the diffusive nature of the filter implies that any non-physical transport between scales is being introduced and (iii) a filtered divergence-free vector remains 'almost' incompressible. Moreover, since they are only based on the diffusive operator, their implementation becomes straightforward. Then, the exact coefficients,  $d_m$ , follow from the requirement that the damping of all the triadic interactions at the smallest scale, must be virtually independent of the  $q$ th Fourier-mode, i.e.  $f_n(\hat{G}_\pi, q) \approx f_n(\hat{G}_\pi)$ . The latter is a crucial property to control the subtle balance between convection and diffusion in order to stop the vortex-stretching mechanism.

The performance of the method has been tested for a Burgers' equation at Reynolds number 100. In this case, the basic 3-point filter ( $M = 1$ ) is not able to control the balance between convection and diffusion at the smallest grid scale. As a consequence, part of the energy is reflected back affecting negatively the numerical solution. This effect is mitigated when using the 5-point ( $M = 2$ ) and the 7-point ( $M = 3$ ) filters. These filters have been constructed to minimize the bandwidth of the damping function. Doing so, the production of small scales of motion is effectively restrained. As expected, the 7-point filter outperforms the 5-point filter only for very coarse meshes.

Finally, it must be noted that apart from  $\mathcal{C}_n$ -regularization modeling, the idea of constructing filters as a function of the discrete diffusive operator can also be used for other applications. Then, depending on the specific application the convolution kernel of the filter would be adjusted via the degrees of freedom, i.e.  $d_1, d_2, d_3$ , etc. For instance, several techniques and subgrid models for LES make use of a test filter [13,14]. The proposed family of discrete linear filters commutes with the differentiation operator. In the context of LES this is a crucial property to ensure that LES equations have the same form as the unfiltered NS equations [15,16]. Together with this, symmetry and normalization are required in LES to guarantee that the filtered equations conserve momentum and dissipate kinetic energy [17]. Therefore, filters defined as in Eq. (23) may be a suitable approach also for LES applications. Moreover, the non-dispersive nature of the proposed filters may make them suitable for other applications. For instance, in the context of Computational AeroAcoustics spurious short waves need to be eliminated. To do so, a common strategy lies in explicitly filtering them without affecting the physical long waves. Suitable filters for such application must minimize dispersion [18]. Hence, the proposed family of filters may also be a good candidate for such application.

## Acknowledgments

This work has been financially supported by the *Ministerio de Educación y Ciencia*, Spain (Project: "Development of high performance parallel codes for the optimal design of thermal equipments". Contract/Grant No. ENE2007-67185), a postdoctoral fellowship *Beatriz de Pinós* (2006 BP-A 10075) by the *Generalitat de Catalunya* and a *Juan de la Cierva* postdoctoral contract (JCI-2009-04910) by the *Ministerio de Ciencia e Innovación*. Authors also wish to thank Dr. I. Jónás for her helpful comments and advices.

## Appendix A. Minimizing the bandwidth of $f_4$

In Section 4.2, it is shown that for the basic 3-point filter the coefficient  $d_1$  is completely determined by Eq. (26) and therefore the bandwidth of  $f_4^{3p}(\hat{G}_\pi, q)$  is fixed (see Fig. 2, also). To solve this more degrees of freedom are needed. Here, we consider to deter-

mine the coefficients  $d_m$  of Eq. (23) with  $M \leq 3$ , that is up to a 7-point filter, from the requirement that the bandwidth of the damping function of the  $\mathcal{C}_4$ -approximation at the smallest grid scale,  $f_4(\hat{G}_\pi, q)$ , must be minimal.

### A.1. 5-point filter

Using a 5-point filter, the associated transfer function (24) yields

$$\hat{G}_k = 1 + d_1 \hat{D}_k + d_2 \hat{D}_k^2, \quad (40)$$

then, plugging the transfer function of the diffusive operator (25) leads to

$$\hat{G}_k = 1 - 2d_1 + 6d_2 + (2d_1 - 8d_2) \cos(k) + 2d_2 \cos(2k). \quad (41)$$

In this case,  $\hat{G}_\pi$  is given by  $\hat{G}_\pi = 1 - 4d_1 + 16d_2$ , and therefore an additional degree of freedom in the coefficients is obtained. This can be used to minimize the bandwidth of the  $f_4^{5p}$  function. Rearranging terms the following expression is obtained

$$f_4^{5p}(\hat{G}_\pi, q, d_2) = a_0(\hat{G}_\pi, d_2) + a_1(\hat{G}_\pi, d_2) \cos(2q) + a_2(\hat{G}_\pi, d_2) \cos(4q), \quad (42)$$

where

$$a_0(\hat{G}_\pi, d_2) = d_2^2 \left( -12\hat{G}_\pi + 6 \right) + d_2 \left( 4\hat{G}_\pi^2 - 2\hat{G}_\pi - 2 \right) + \left( -\frac{1}{4}\hat{G}_\pi^3 - \frac{3}{8}\hat{G}_\pi^2 + \frac{3}{2}\hat{G}_\pi + \frac{1}{8} \right), \quad (43a)$$

$$a_1(\hat{G}_\pi, d_2) = d_2^2 \left( 16\hat{G}_\pi - 8 \right) + d_2 \left( -4\hat{G}_\pi^2 + 2\hat{G}_\pi + 2 \right) + \left( \frac{1}{4}\hat{G}_\pi^3 - \frac{5}{8}\hat{G}_\pi^2 + \frac{1}{2}\hat{G}_\pi - \frac{1}{8} \right), \quad (43b)$$

$$a_2(\hat{G}_\pi, d_2) = d_2^2 \left( -4\hat{G}_\pi + 2 \right). \quad (43c)$$

Furthermore,  $f_4^{5p}(\hat{G}_\pi, q, d_2)$  is bounded by  $q = 0, q = \pi/2$  and  $q = 1/2 \cos^{-1}(-a_1/4a_2)$ ,

$$f_4^{5p}(\hat{G}_\pi, 0, d_2) = a_0 + a_1 + a_2 \quad (44a)$$

$$f_4^{5p}(\hat{G}_\pi, \pi/2, d_2) = a_0 - a_1 + a_2 \quad (44b)$$

$$f_4^{5p}(\hat{G}_\pi, 1/2 \cos^{-1}(-a_1/4a_2), d_2) = a_0 - a_2 - \frac{a_1^2}{8a_2} \quad (44c)$$

where the latter is a proper value only for values of  $d_2$  satisfying  $|a_1| \leq 4a_2$ . Then, choosing  $d_2$  with the criterion that  $a_1 = -4a_2$  leads to

$$d_{1,opt} = -\frac{\hat{G}_\pi - 1}{2(2\hat{G}_\pi + 1)} \text{ and } d_{2,opt} = \frac{2\hat{G}_\pi^2 - 3\hat{G}_\pi + 1}{16(2\hat{G}_\pi + 1)}. \quad (45)$$

Therefore, the values of  $f_4^{5p}$  for  $q = 1/2 \cos^{-1}(-a_1/4a_2)$  and  $q = 0$  coincide and  $f_4^{5p}$  remains positive for all  $p, q$  at  $\hat{G}_\pi = 0$ . Hence, for  $d_2 = d_{2,opt}$   $f_4$  is again bounded by  $q = 0$  and  $q = \pi/2$ . Fig. 3 (top) shows the bandwidth of  $f_4^{5p}(\hat{G}_\pi, q, d_{2,opt})$  for  $0 \leq \hat{G}_\pi \leq 1$ .

### A.2. 7-point filter

However, the bandwidth of  $f_4^{5p}$  for low values of  $\hat{G}_\pi$  is still significant. To minimize it we propose to use the 7-point filter

$$\hat{G}_k = 1 + d_1 \hat{D}_k + d_2 \hat{D}_k^2 + d_3 \hat{D}_k^3, \quad (46)$$

then, substituting the transfer function of the diffusive operator (25) leads to

$$\hat{G}_k = 1 - 2d_1 + 6d_2 - 20d_3 + (2d_1 - 8d_2 + 30d_3) \cos(k) + (2d_2 - 12d_3) \cos(2k) + 2d_3 \cos(3k). \quad (47)$$

In this case,  $\hat{G}_\pi = 1 - 4d_1 + 16d_2 - 64d_3$  and therefore we have two degrees of freedom

$$f_4^{7p}(\hat{G}_\pi, q, d_2, d_3) = a_0(\hat{G}_\pi, d_2, d_3) + a_1(\hat{G}_\pi, d_2, d_3) \cos(2q) \\ + a_2(\hat{G}_\pi, d_2, d_3) \cos(4q) + a_3(\hat{G}_\pi, d_2, d_3) \cos(6q), \quad (48)$$

where

$$a_0(\hat{G}_\pi, d_2, d_3) = d_2^2(-12\hat{G}_\pi + 6) + d_3^2(-424\hat{G}_\pi + 212) \\ + d_2 d_3(144\hat{G}_\pi - 72) + d_2(4\hat{G}_\pi^2 - 2\hat{G}_\pi - 2) \\ + d_3(-22\hat{G}_\pi^2 + 9\hat{G}_\pi + 13) - \frac{1}{4}\hat{G}_\pi^3 - \frac{3}{8}\hat{G}_\pi^2 \\ + \frac{3}{2}\hat{G}_\pi + \frac{1}{8}, \quad (49)$$

$$a_1(\hat{G}_\pi, d_2, d_3) = d_2^2(16\hat{G}_\pi - 8) + d_3^2(572\hat{G}_\pi - 286) \\ + d_2 d_3(-192\hat{G}_\pi + 96) + d_2(-4\hat{G}_\pi^2 + 2\hat{G}_\pi + 2) \\ + d_3(24\hat{G}_\pi^2 - 12\hat{G}_\pi - 12) + \frac{1}{4}\hat{G}_\pi^3 - \frac{5}{8}\hat{G}_\pi^2 + \frac{1}{2}\hat{G}_\pi - \frac{1}{8}, \quad (50)$$

$$a_2(\hat{G}_\pi, d_2, d_3) = d_2^2(-4\hat{G}_\pi + 2) + d_3^2(-152\hat{G}_\pi + 76) \\ + d_2 d_3(48\hat{G}_\pi - 24) + d_3(-2\hat{G}_\pi^2 + 3\hat{G}_\pi - 1), \quad (51)$$

$$a_3(\hat{G}_\pi, d_2, d_3) = d_3^2(4\hat{G}_\pi - 2). \quad (52)$$

Then, the optimal values for  $d_2$  and  $d_3$  are given by the following equation

$$\frac{d}{dq} f_4^{7p}(q) = -2a_1 \sin(2q) - 4a_2 \sin(4q) - 6a_3 \sin(6q) = 0. \quad (53)$$

Applying the double-angle formula,  $\sin(2\alpha) = 2\sin(\alpha)\cos(\alpha)$ , and the triple-angle formula,  $\sin(3\alpha) = 3\sin(\alpha) - 4\sin^3(\alpha)$ , leads to

$$\frac{d}{dq} f_4^{7p}(q) = \sin(2q)[-2a_1 - 8a_2 \cos(2q) - 18a_3 + 24a_3 \sin^2(2q)] = 0, \quad (54)$$

and therefore, zeros are given by

$$\sin(2q) = 0, \quad (55)$$

$$-2a_1 - 8a_2 \cos(2q) - 18a_3 + 24a_3 \sin^2(2q) = 0. \quad (56)$$

Thus, the roots of the first equation are  $q_1 = 0$  and  $q_2 = \pi/2$ . Then, rest of roots are given by Eq. (56). Using the Pythagorean trigonometric identity,  $\sin^2(\alpha) + \cos^2(\alpha) = 1$ , we obtain a quadratic equation for  $\cos(2q)$

$$-24a_3 \cos^2(2q) - 8a_2 \cos(2q) + (-2a_1 + 6a_3) = 0, \quad (57)$$

which roots are given by

$$\cos(2q) = \frac{1}{6} \frac{-a_2 \pm \sqrt{a_2^2 - 3a_1 a_3 + 9a_3^2}}{a_3}. \quad (58)$$

Then, a proper bound is given by the following equation

$$\frac{1}{6} \frac{-a_2 \pm \sqrt{a_2^2 - 3a_1 a_3 + 9a_3^2}}{a_3} = \pm \frac{1}{2}. \quad (59)$$

Therefore, the rest of roots is given by  $q_3 = \pi/6$  and  $q_4 = \pi/3$ . Then, to fulfill the previous equation, the following equations must be satisfied

$$a_2 = 0, \quad (60)$$

$$a_1 = 0. \quad (61)$$

Imposing the first Eq. (60) leads to

$$d_2 = 6d_3 \pm \frac{1}{2} \sqrt{-8d_3^2 - 2d_3 \hat{G}_\pi + 2d_3}; \quad (62)$$

however, only the solution

$$d_{2,opt} = 6d_3 + \frac{1}{2} \sqrt{-8d_3^2 - 2d_3 \hat{G}_\pi + 2d_3}, \quad (63)$$

guarantees  $d_2 > 0$ . Then, two solutions for  $d_3$  follow from Eq. (61). However, proper bounds are only given by

$$d_{3,opt} = \frac{1}{54} \left( \frac{E(\hat{G}_\pi)}{C(\hat{G}_\pi)} + \frac{D(\hat{G}_\pi)}{E(\hat{G}_\pi)} - \frac{7}{2} \right) (\hat{G}_\pi - 1), \quad (64)$$

where

$$C(\hat{G}_\pi) = 4\hat{G}_\pi^2 - 4\hat{G}_\pi + 1, \quad (65a)$$

$$D(\hat{G}_\pi) = 4\hat{G}_\pi^2 - 196\hat{G}_\pi + 1, \quad (65b)$$

$$E(\hat{G}_\pi) = \left( C^2(\hat{G}_\pi) \left( A(\hat{G}_\pi) + 12\sqrt{6} \sqrt{\hat{G}_\pi B(\hat{G}_\pi)/C(\hat{G}_\pi)} \right) \right)^{1/3}, \quad (65c)$$

with  $A(\hat{G}_\pi) = 4\hat{G}_\pi^2 + 1004\hat{G}_\pi + 1$  and  $B(\hat{G}_\pi) = 48\hat{G}_\pi^4 + 4096\hat{G}_\pi^3 + 4072\hat{G}_\pi^2 + 1024\hat{G}_\pi + 3$ . In summary, the values of optimal values for  $d_1$ ,  $d_2$ ,  $d_3$  are given by

$$d_{3,opt} = \frac{1}{54} \left( \frac{E(\hat{G}_\pi)}{C(\hat{G}_\pi)} + \frac{D(\hat{G}_\pi)}{E(\hat{G}_\pi)} - \frac{7}{2} \right) (\hat{G}_\pi - 1), \quad \text{if } 0 \leq \hat{G}_\pi < 1/2 \quad (66)$$

$$d_{3,opt} = 0, \quad \text{if } 1/2 \leq \hat{G}_\pi \leq 1 \quad (67)$$

then, optimal values for  $d_2$  and  $d_1$  follow from Eqs. (63) and (47), respectively

$$d_{2,opt} = 6d_{3,opt} + \frac{1}{2} \sqrt{-8d_{3,opt}^2 - 2d_{3,opt} \hat{G}_\pi + 2d_{3,opt}} \quad \text{if } 0 \leq \hat{G}_\pi < 1/2 \quad (68)$$

$$d_{2,opt} = \frac{2\hat{G}_\pi^2 - 3\hat{G}_\pi + 1}{16(2\hat{G}_\pi + 1)}, \quad \text{if } 1/2 \leq \hat{G}_\pi \leq 1 \quad (69)$$

and

$$d_{1,opt} = \frac{1}{4} (1 + 16d_{2,opt} - 64d_{3,opt} - \hat{G}_\pi), \quad \text{if } 0 \leq \hat{G}_\pi < 1/2 \quad (70)$$

$$d_{1,opt} = -\frac{\hat{G}_\pi - 1}{2(2\hat{G}_\pi + 1)}, \quad \text{if } 1/2 \leq \hat{G}_\pi \leq 1 \quad (71)$$

Therefore, for  $\hat{G}_\pi \geq 1/2$ , it becomes again the 5-point filter. Actually, the transition from  $f_4^{5p}$  to  $f_4^{7p}$  at  $\hat{G}_\pi = 1/2$  is smooth.<sup>2</sup> Moreover, since the expression for  $f_4^{7p}$  reduces to

$$f_4^{7p}(\hat{G}_\pi, q, d_{2,opt}, d_{3,opt}) = a_0 - 3a_3 \cos(2q) + 4a_3 \cos^3(2q), \quad (72)$$

the values of  $f_4^{7p}$  for  $q_3 = \pi/6$  and  $q_4 = \pi/3$  coincide with  $q_1 = \pi/2$  and  $q_2 = 0$ , respectively. Hence, for  $d_{3,opt}$ ,  $d_{2,opt}$ ,  $d_{1,opt}$ ,  $f_4$  is again bounded by  $q = 0$  and  $q = \pi/2$ . Fig. 3 (bottom) shows the bandwidth of  $f_4^{7p}(\hat{G}_\pi, q, d_{2,opt}, d_{3,opt})$  for  $0 \leq \hat{G}_\pi \leq 1$ .

### A.3. Constructing filters for $\mathcal{C}_2$

The same analysis can be applied for the  $\mathcal{C}_2$  regularization given by Eq. (7a). In this case,  $f_2(\hat{G}_\pi, \hat{G}_p, \hat{G}_q) = \hat{G}_\pi \hat{G}_p \hat{G}_q$  and therefore the damping function  $f_2^{3p}$  for the 3-point filter becomes

$$f_2^{3p}(\hat{G}_\pi, q) = \frac{1}{8} \hat{G}_\pi^3 + \frac{3}{4} \hat{G}_\pi^2 + \frac{1}{8} \hat{G}_\pi + \left( -\frac{1}{8} \hat{G}_\pi^3 + \frac{1}{4} \hat{G}_\pi^2 - \frac{1}{8} \hat{G}_\pi \right) \cos(2q), \quad (73)$$

which is bounded by  $f_2^{3p}(\hat{G}_\pi, 0)$  and  $f_2^{3p}(\hat{G}_\pi, \pi/2)$

<sup>2</sup> Actually at  $\hat{G}_\pi = 1/2$ ,  $d_{3,opt} = 0$ . However, it must be noted that  $\lim_{\hat{G}_\pi \rightarrow 1/2} C(\hat{G}_\pi) = 0$  and  $\lim_{\hat{G}_\pi \rightarrow 1/2} E(\hat{G}_\pi) = 0$ . Hence, special care must be taken when evaluating  $d_{3,opt}$  for values close to  $\hat{G}_\pi = 1/2$ .

$$f_2^{3p}(\hat{G}_\pi, 0) = \hat{G}_\pi^2, \quad (74)$$

$$f_2^{3p}(\hat{G}_\pi, \pi/2) = \frac{1}{4}\hat{G}_\pi^3 + \frac{1}{2}\hat{G}_\pi^2 + \frac{1}{4}\hat{G}_\pi. \quad (75)$$

Since for the 3-point filter, the coefficient  $d_1$  is given by the condition (26), the bandwidth is fixed. Again, the bandwidth of  $f_2$  can be minimized by adding additional degrees of freedom in the coefficients. Using a 5-point filter the damping function for  $\mathcal{G}_2$  reads

$$f_2^{5p}(\hat{G}_\pi, q, d_2) = a_0(\hat{G}_\pi, d_2) + a_1(\hat{G}_\pi, d_2) \cos(2q) + a_2(\hat{G}_\pi, d_2) \cos(4q), \quad (76)$$

where

$$a_0(\hat{G}_\pi, d_2) = d_2^2(6\hat{G}_\pi) + d_2(-2\hat{G}_\pi^2 - 2\hat{G}_\pi) + \left(\frac{1}{8}\hat{G}_\pi^3 + \frac{3}{4}\hat{G}_\pi^2 + \frac{1}{8}\hat{G}_\pi\right), \quad (77)$$

$$a_1(\hat{G}_\pi, d_2) = d_2^2(-8\hat{G}_\pi) + d_2(2\hat{G}_\pi^2 + 2\hat{G}_\pi) + \left(-\frac{1}{8}\hat{G}_\pi^3 + \frac{1}{4}\hat{G}_\pi^2 - \frac{1}{8}\hat{G}_\pi\right), \quad (78)$$

$$a_2(\hat{G}_\pi, d_2) = d_2^2(2\hat{G}_\pi). \quad (79)$$

Furthermore,  $f_2^{5p}(\hat{G}_\pi, q, d_2)$  is bounded by  $q = 0$ ,  $q = \pi/2$  and  $q = 1/2 \cos^{-1}(-a_1/4a_2)$ ,

$$f_2^{5p}(\hat{G}_\pi, 0, d_2) = a_0 + a_1 + a_2, \quad (80)$$

$$f_2^{5p}(\hat{G}_\pi, \pi/2, d_2) = a_0 - a_1 + a_2, \quad (81)$$

$$f_2^{5p}(\hat{G}_\pi, 1/2 \cos^{-1}(-a_1/4a_2), d_2) = a_0 - a_2 - \frac{a_1^2}{8a_2}, \quad (82)$$

where the latter is a proper value only for values of  $d_2$  satisfying  $|a_1| \leq 4a_2$ . Then, choosing  $d_2$  with the criterion that  $a_1 = -4a_2$  leads to

$$d_{2,opt} = \frac{\hat{G}_\pi^2 - 2\hat{G}_\pi + 1}{16(\hat{G}_\pi + 1)} \text{ and } d_{1,opt} = -\frac{\hat{G}_\pi - 1}{2(\hat{G}_\pi + 1)}. \quad (83)$$

Finally, using a 7-point filter the bandwidth of  $f_2$  can be further reduced. In this case, the damping function of  $\mathcal{G}_2$  reads

$$f_2^{7p}(\hat{G}_\pi, q, d_2, d_3) = (a_0 - a_2) + (a_1 - 3a_3) \cos(2q) + 2a_2 \cos^2(2q) + 4a_3 \cos^3(2q), \quad (84)$$

where

$$a_0(\hat{G}_\pi, d_2, d_3) = d_2^2(6\hat{G}_\pi) + d_3^2(212\hat{G}_\pi) + d_2d_3(-72\hat{G}_\pi) + d_2(-2\hat{G}_\pi^2 - 2\hat{G}_\pi) + d_3(11\hat{G}_\pi^2 + 13\hat{G}_\pi) + \left(\frac{1}{8}\hat{G}_\pi^3 + \frac{3}{4}\hat{G}_\pi^2 + \frac{1}{8}\hat{G}_\pi\right), \quad (85)$$

$$a_1(\hat{G}_\pi, d_2, d_3) = d_2^2(-8\hat{G}_\pi) + d_3^2(-286\hat{G}_\pi) + d_2d_3(96\hat{G}_\pi) + d_2(2\hat{G}_\pi^2 + 2\hat{G}_\pi) + d_3(-12\hat{G}_\pi^2 - 12\hat{G}_\pi) + \left(-\frac{1}{8}\hat{G}_\pi^3 + \frac{1}{4}\hat{G}_\pi^2 - \frac{1}{8}\hat{G}_\pi\right), \quad (86)$$

$$a_2(\hat{G}_\pi, d_2, d_3) = d_2^2(2\hat{G}_\pi) + d_3^2(76\hat{G}_\pi) + d_2d_3(-24\hat{G}_\pi) + d_3(\hat{G}_\pi^2 - \hat{G}_\pi), \quad (87)$$

$$a_3(\hat{G}_\pi, d_2, d_3) = d_3^2(-2\hat{G}_\pi). \quad (88)$$

Then, repeating the same reasoning leads again to Eqs. (60) and (61). This leads to the following solution

$$d_{1,opt} = \frac{1}{4}(1 + 16d_{2,opt} - 64d_{3,opt} - \hat{G}_\pi) \quad (89)$$

$$d_{2,opt} = 6d_{3,opt} + \frac{1}{2}\sqrt{-8d_{3,opt}^2 - 2d_{3,opt}\hat{G}_\pi + 2d_{3,opt}} \quad (90)$$

$$d_{3,opt} = \frac{1}{54}\left(K(\hat{G}_\pi) - \frac{J(\hat{G}_\pi)}{K(\hat{G}_\pi)} - \frac{7}{2}(\hat{G}_\pi - 1)\right) \quad (91)$$

where  $J(\hat{G}_\pi) = -\hat{G}_\pi^2 + 98\hat{G}_\pi - 1$  and  $K(\hat{G}_\pi) = (F(\hat{G}_\pi) + 12\sqrt{H(\hat{G}_\pi)})^{1/3}$  with  $F(\hat{G}_\pi) = \hat{G}_\pi^3 + 501\hat{G}_\pi^2 - 501\hat{G}_\pi - 1$  and  $H(\hat{G}_\pi) = 9\hat{G}_\pi^5 + 1536\hat{G}_\pi^4 + 3054\hat{G}_\pi^3 + 1536\hat{G}_\pi^2 + 9\hat{G}_\pi$ , respectively.

## References

- [1] Verstappen RWCP, Veldman AEP. Symmetry-preserving discretization of turbulent flow. *J Comput Phys* 2003;187:343–68.
- [2] Guemond JL, Oden JT, Prudhomme S. Mathematical perspectives on large eddy simulation models for turbulent flows. *J Math Fluid Mech* 2004;6:194–248.
- [3] Geurts BJ, Holm DD. Regularization modeling for large-eddy simulation. *Phys Fluids* 2003;15:L13–6.
- [4] Leray J. Sur le mouvement d'un liquide visqueux emplissant l'espace. *Acta Math* 1934;63:193–248.
- [5] Verstappen R. On restraining the production of small scales of motion in a turbulent channel flow. *Comput Fluids* 2008;37:887–97.
- [6] Trias FX, Soria M, Oliva A, Verstappen RWCP. Regularization models for the simulation of turbulence in a differentially heated cavity. In: *Proceedings of the European computational fluid dynamics conference (ECCOMAS CFD 2006)*, Egmond aan Zee, The Netherlands; 2006.
- [7] Trias FX, Verstappen RWCP, Gorobets A, Soria M, Oliva A. Parameter-free symmetry-preserving regularization modeling of a turbulent differentially heated cavity. *Comput Fluids* [published online] 2010;39:1815–31.
- [8] Carati D, Winckelmans GS, Jeanmart H. Exact expansions for filtered-scales modelling with a wide class of LES filters. In: *Direct and large-eddy simulation III*. Kluwer; 1999. p. 213–24.
- [9] Mahesh K, Constantinescu G, Moin P. A numerical method for large-eddy simulation in complex geometries. *J Comput Phys* 2004;197:215–40.
- [10] van Reeuwijk M, Jonker HJJ, Hanjalić K. Incompressibility of the Leray- $\alpha$  model for wall-bounded flows. *Phys Fluids* 2006;18(1):018103.
- [11] Basu S. Can the dynamic eddy-viscosity class of subgrid-scale models capture inertial-range properties of Burgers turbulence? *J Turbul* 2009;10(12):1–16.
- [12] Helder J, Verstappen R. On restraining convective subgrid-scale production in Burgers' equation. *Int J Numer Methods Fluids* 2008;56(8):1289–95.
- [13] Sagaut P, Grohens R. Discrete filters for large eddy simulations. *Int J Numer Methods Fluids* 1999;31:1195–220.
- [14] Sagaut P. Large eddy simulation for incompressible flows: an introduction. 3rd ed. Springer; 2005.
- [15] Vasilyev OV, Lund TS, Moin P. A general class of commutative filters for LES in complex geometries. *J Comput Phys* 1998;146(1):82–104.
- [16] Marsden AL, Vasilyev OV, Moin P. Construction of commutative filters for LES on unstructured meshes. *J Comput Phys* 2002;175(2):584–603.
- [17] Vreman AW. The adjoint filter operator in large-eddy simulation of turbulent flow. *Phys Fluids* 2004;16:2012–22.
- [18] Bogey C, Bailly C. A family of low dispersive and low dissipative explicit schemes for flow and noise computations. *J Comput Phys* 2004;194(1):194–214.